ANALYSIS OF THE FAR IR SPECTRUM OF TRIMETHYLENE SULFIDE USING EVOLUTIONARY ALGORITHMS

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Rotationally-resolved vibrational spectra have been collected from 100-1000 cm^{-1} for the four-membered ring trimethylene sulfide (c-C_3H_6S) using synchrotron light at the far infrared beamline of the Canadian Light Source. The spectra are complicated by the presence of ring inversion tunneling which gives rise to dense patterns of overlapping rotation-vibration-inversion transitions in the infrared region. These are well-resolved using the Bruker IFS125HR instrument. In this talk, we will discuss the progress of the analysis of the two lowest frequency bands which correspond to the *c*-type ring puckering vibration at 139 cm^{-1}, and the *a*-type in-plane ring deformation at 529 cm^{-1}. The ideas of genetic evolution via evolutionary strategies have been used to aid in the analysis of the observed spectra. In particular, we have applied the covariance matrix adaptation evolution strategy which uses the concept of mutation and the results of previous trials to give solutions to fit the quite dense spectra.